OUTLINE FOR CHEMISTRY 580
FALL 2020: TR 9:30 – 10:45 AM: Online

Instructor: Mark Gordon, 201 Spedding
Office Hours, 11-12 Noon TR, or by arrangement
Text: F. Jensen, "Introduction to Computational Chemistry", 3rd Edition, Wiley

NOTE: All cell phones and smart phones MUST be turned off during class. No texting or talking on phones.

I. Background: From Schrodinger to Hartree and Fock
- A. Introduction to Schrodinger Equation
- B. Roadblocks and need for the orbital approximation
- C. The orbital and Hartree-Fock approximations
- D. The LCAO-MO approximation
- E. Density Functional Theory
- F. Electron Correlation: Beyond Hartree-Fock

II. Hands-on applications (using GAMESS, graphics, other codes)

It will be assumed that students have a working knowledge of point groups
- A. Basis sets
- B. Predictions of molecular properties
- C. Finding transition states and reaction paths
- D. Solvent Effects
- E. Fragmentation methods
- F. **Choosing Class Project Deadline**

III. Hybrid and semi-empirical molecular orbital methods:
- A. Hybrid methods (G2, G3, other composite methods)
- B. Introduction to ZDO methods
- C. Commonly used semi-empirical methods
- D. Molecular Mechanics, QM/MM methods
- F. Applications and reality checks

Grade is based on:

Mid-Term (take-home): 40%
Paper on Class Project: 40%
Seminar on Class Project: 20%

Class Project: The class project will involve an application of computational chemistry to a project that is relevant to the student's research interests.

Persons with disabilities: Please address any special needs or special accommodations with me at the beginning of the semester or as soon as you become aware of your needs. Those seeking accommodations based on disabilities should obtain a Student Academic Accommodation Request (SAAR) form from the Student Disability Resource (SDR) office (phone 515-294-7220). SDR is located on the main floor of the Student Services Building, Room 1076.